

Quantum phase transition in the sub-Ohmic spin-boson model

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We study systematically the quantum phase transition (QPT) of the sub-Ohmic spin-boson model (SBM) in the full range of the power index s of the spectral density. Under the rotating-wave approximation (RWA), it is found that the usual delocalized-localized QPT is absent but a novel QPT occurs, which can be deduced analytically from whether a bound state between the spin and its reservoir exists or not. Surprisingly, this QPT has been missed in the literature for a long time. When the RWA is relaxed, the delocalized-localized QPT is recovered by using a unitary transformation plus perturbation method. Meanwhile, the novel QPT found under the RWA still exists but is located in the delocalized phase regime. In both cases the novel QPT causes a dynamical transition of the spin system from complete decoherence to decoherence suppression, which suggests a useful control way to the detrimental effects of the reservoir to the system. The result also implies that the coherent-incoherent transition studied extensively in the literature is caused essentially by the intrinsic QPT of the system.

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I. INTRODUCTION

Quantum phase transition (QPT), occurring at the absolute zero temperature, is induced by varying the external temperature-independent parameters, which results in a sudden qualitative change of the macroscopic properties mapped from the eigen-spectrum of a quantum many-body system [1]. Recently, there are intense interests in QPT of a small quantum system coupled to a dissipative reservoir, e.g. the spin-boson model (SBM) and the Dicke model [2]. The SBM describes an effective two-level system (TLS) interacting with a collection of harmonic oscillators acting as the bosonic reservoir. The effect of the reservoir is characterized by the spectral density $J(\omega)$, which is phenomenologically described by the power law to the frequency of the reservoir, i.e. $J(\omega) \propto \omega^s$. The renewed interest in the SBM arises from the fact that the interaction of the TLS as a qubit with its reservoir leads to the decoherence which is a main obstacle to implement quantum information processing [3]. One desires that the exploration the QPT in the SBM can supply some insight to the decoherence control of the qubit system. A variety of approximate analytical and numerical methods, for example path integral method under non-interacting blip approximation [4], variational method based on unitary transformation [5, 6], numerical renormalization group method [7], quantum Monte Carlo method [8], and numerical diagonalization in coherent-state basis [9], have been developed. A consensus is that the SBM shows a QPT from delocalization to localization with the increase of the dimensionless coupling constant

in the Ohmic case ($s = 1$), as a consequence of the competition between the internal tunneling effect of the TLS and the external dissipation effect of the reservoir.

The QPT of the SBM in sub-Ohmic case ($0 < s < 1$) has attracted much attention recently. One of the motivations originates from the idea that the sub-Ohmic reservoir can be used to model $1/f$ noise [10], which is the main source of decoherence in solid state systems, e.g. quantum dots [11, 12] and superconductor qubit systems [13, 14]. Another motivation is that the sub-Ohmic SBM is more involved than the Ohmic case. Different methods to the sub-Ohmic SBM can even not lead to a qualitatively consistent result. The path integral method under non-interacting blip approximation predicts that the QPT from delocalization to localization is absent for the sub-Ohmic SBM [4]. The numerical renormalization group method confirms the occurrence of the QPT in the full range $0 < s < 1$, while the breakdown of the quantum-to-classical mapping for $0 < s < 1/2$ [7], which means the failure of the classical mean-field description to the QPT. However, the quantum Monte Carlo method and the numerical diagonalization in coherent-state basis predict the presence of the QPT, the well-defined quantum-to-classical mapping, and the classical critical exponents to the sub-Ohmic SBM [8, 9].

While the physics in the localized regime of the SBM is trivial, the delocalized regime exhibits many interesting phenomena. For example, it was shown that the dynamics of the spin in the delocalized regime changes from the damped coherent oscillation to incoherent relaxation with the increase of the coupling strength for both of the Ohmic [4] and the sub-Ohmic [15–17] SBM. This dynamical phenomenon is named as the coherent-incoherent transition [4]. What is the physical reason of this dynamical transition? As a dynamical behavior, it does

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not suffice to deduce the occurrence of the intrinsic QPT of the model because it is initial-state-dependent. By evaluating the ground-state energy of the Ohmic SBM, it was shown in Ref. [18] that the coherent-incoherent transition is actually the dynamical consequence of another intrinsic QPT occurred in the delocalized regime.

In the present work, we study the ground state energy and the dynamics of the TLS of the sub-Ohmic SBM both with and without the rotating-wave approximation (RWA). Under the RWA, we find analytically that a novel QPT occurs in the full range of the sub-Ohmic spectrum, while the delocalized-localized QPT is absent. This QPT separates the dynamics of the TLS into complete decoherence and decoherence suppression. When the RWA is relaxed, using the perturbation approach based on a unitary transformation, which has been successfully used to capture the delocalized-localized QPT for the Ohmic [5, 6] and the sub-Ohmic [17] SBM, we find that the novel QPT happened explicitly in the conventional delocalized phase regime still exists. It implies that besides the conventional delocalized-localized QPT, there is another QPT in the SBM. The compatibility of the novel QPT with the coherent-incoherent transition makes us conjecture that the coherent-incoherent transition occurring in the delocalized regime is actually caused by an intrinsic QPT. Our analytical formulation provides a clear physical picture of this QPT and a unified description of the QPT in the sub-Ohmic SBM.

This paper is organized as follows. In Sec. II, the SBM and its simplification under the RWA are introduced. To illustrate the new kind of QPT, we explore in Sec. III the QPT in the SBM under the RWA by examining the formation of a bound state. In Sec. IV, the QPT in the sub-Ohmic SBM is investigated by means of the perturbation approach based on a unitary transformation [5, 6]. A novel QPT is found in the usual delocalized phase regime. Sec. V is devoted to the dynamical consequence of such QPT. Finally, a brief discussion and summary are given in Sec. VI.

II. THE MODEL

The SBM, which relates to a variety of physical and chemical processes [19], describes the tunneling of a quantum particle in a double well potential under the influence of a bosonic reservoir. Its Hamiltonian reads

$$\hat{H} = \frac{\epsilon}{2}\hat{\sigma}_z - \frac{\Delta}{2}\hat{\sigma}_x + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k \frac{g_k}{2} \hat{\sigma}_z (\hat{b}_k + \hat{b}_k^\dagger), \quad (1)$$

where ϵ is the difference between the two energy levels in the wells, Δ is the tunneling amplitude between the two wells, \hat{b}_k^\dagger and \hat{b}_k are, respectively, the creation and annihilation operators of k -th mode of the reservoir with frequency ω_k . The coupling strength between the particle and its reservoir is denoted by g_k , which is further characterized by the spectral density $J(\omega) =$

$\pi \sum_k |g_k|^2 \delta(\omega - \omega_k)$. In the continuum limit the spectral density may have the form

$$J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s\Theta(\omega_c - \omega), \quad (2)$$

where α is a dimensionless coupling constant, ω_c is a cutoff frequency, and $\Theta(x)$ is the usual step function. The reservoir is classified as Ohmic when $s = 1$, sub-Ohmic when $0 < s < 1$, and super-Ohmic when $s > 1$ [4]. In spite of the simplicity of its formulation, the SBM does not admit an exact solution in a closed analytical form and one often resorts to numerical simulations or various approximations for its analysis. Under a unitary transformation $\hat{U}_1 = \exp(-i\pi\hat{\sigma}_y/4)$, one can prove that Eq. (1) is equivalent to

$$\hat{H}_z = \frac{\epsilon}{2}\hat{\sigma}_x + \frac{\Delta}{2}\hat{\sigma}_z + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k \frac{g_k}{2} \hat{\sigma}_x (\hat{b}_k + \hat{b}_k^\dagger), \quad (3)$$

which corresponds to a $\pi/4$ -rotation around $\hat{\sigma}_y$ to SBM (1). In the following, we assume $\epsilon = 0$, which corresponds to the case of the un-biased double potential wells where there has no energy difference between the two wells.

The interaction in Eq. (3) contains the counter rotating terms, $\hat{b}_k^\dagger \hat{\sigma}_+$ and $\hat{b}_k \hat{\sigma}_-$. A widely used approximation in quantum optics and quantum information communities is the RWA, which is applicable in the weak coupling limit. Then Eq. (3) is reduced to

$$\hat{H}_{\text{RWA}} = \frac{\Delta}{2}\hat{\sigma}_z + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k \frac{g_k}{2} (\hat{\sigma}_+ \hat{b}_k + \hat{\sigma}_- \hat{b}_k^\dagger). \quad (4)$$

Eq. (4) is analytically solvable because the total excitation number $\hat{N} = \sum_k \hat{b}_k^\dagger \hat{b}_k + \hat{\sigma}_+ \hat{\sigma}_-$ of the whole system is conserved.

III. QPT UNDER THE RWA

The Hamiltonian (4) under the RWA is widely used to characterize decoherence of a qubit in quantum optics and quantum information communities. It is found that the decoherence dynamics of the TLS in this situation exhibits rich behaviors in different spectral densities of the reservoir, such as the exponential decay under the Born-Markovian approximation [20], the oscillatory decay in a lossy cavity with Lorentzian spectral density [21], even the decoherence suppression in engineered reservoir with photonic band gap structure [22–24]. Further studies show that whether a bound state of the global system is formed or not essentially plays a key role in such rich dynamical behaviors [25–27]. Experimentally, the bound-state induced decoherence suppression has been observed [28–30]. In this section, starting from Eq. (4), we investigate analytically and numerically QPT via examining the formation of a bound state between the TLS and its reservoir. We reveal that the formation of the bound state actually implies a QPT of the system.

A. Analytical results

Since \hat{N} is conserved, the Hilbert space is split into the direct sum of the subspaces with definite quantum number N . In this situation one can naively deem that the eigenstate $|\varphi_0\rangle = |-, \{0_k\}\rangle$, a tensor product of the respective ground states of the two subsystems in zero-excitation subspace with eigenvalue $E_0 = -\Delta/2$, is the ground state of the whole system. Is this always true? To verify this, let us examine the eigen solution of \hat{H}_{RWA} in the single-excitation subspace, which can be expanded as $|\varphi_1\rangle = c_0 |+, \{0_k\}\rangle + \sum_{k=0}^{\infty} c_k |-, 1_k\rangle$. From the eigen-equation governed by Eq. (4) we can obtain a transcendental equation of E_1

$$y(E_1) \equiv \frac{\Delta}{2} - \frac{1}{4\pi} \int_0^{\infty} \frac{J(\omega)}{\omega - (E_1 + \frac{\Delta}{2})} d\omega = E_1. \quad (5)$$

A bound state is an eigenstate with real (discrete) eigenvalue in a quantum many-body system. So if Eq. (5) has real root, we can claim that the system possesses a bound state [26, 31]. We can easily find that $y(E_1)$ decreases monotonically with the increase of E_1 in the regime of $E_1 < -\frac{\Delta}{2}$. Therefore if the condition

$$y(-\frac{\Delta}{2}) \leq -\frac{\Delta}{2}, \quad (6)$$

is satisfied, $y(E_1)$ always has one and only one intersection with the function on the right-hand side of Eq. (5). This root just corresponds to the eigenvalue of the formed bound state in the Hilbert space of the system plus its reservoir. On the other hand, in the regime of $E_1 > -\frac{\Delta}{2}$, we can see that $y(E_1)$ is divergent, which means that no real root E_1 can make Eq. (5) well-defined. Consequently, Eq. (5) does not have real root to support the existence of a further bound state in this regime. It is noted that Eq. (5) may possess complex root. Physically, this means that the corresponding eigenstate experiences decay contributed from the imaginary part of the eigenvalue during the time evolution, which causes the excited-state population approaching zero asymptotically and the decoherence of the TLS. However, to the bound state, the excited-state population is constant in time. This means that the formation of bound state can result in decoherence suppression.

With the formation of the bound state, the ground state is changed from $|\varphi_0\rangle$ to the bound state $|\varphi_1\rangle$, because $E_1 < E_0$. We can verify that the eigenstates of \hat{H}_{RWA} in the subspaces $N \geq 2$ actually have larger eigenvalues than E_1 , which is shown in Appendix A. This implies that the higher-boson states may not become the ground state. One may also observe that the two states are orthogonal, i.e. $\langle -, \{0_k\} | \varphi_1 \rangle = 0$. Therefore, the energy-level crossing accompanying with the formation of bound state signals clearly that the system undergoes a QPT. From the criterion (6), it is readily to evaluate that the QPT happens at the critical point

$$\alpha_{\text{C,RWA}} = \frac{2s\Delta}{\omega_c}, \quad (7)$$

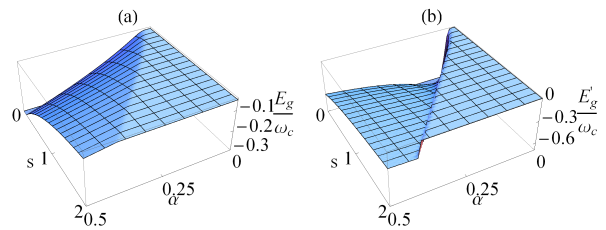


FIG. 1. (Color online) Ground-state energy E_g (a) and its first derivative $E'_g = \frac{\partial E_g}{\partial \alpha}$ (b) as a function of the coupling constant α and power index s of the spectrum. The parameter used here is $\Delta = 0.1\omega_c$. According to Eq. (7), the first-order QPT occurs at $\alpha_{\text{C,RWA}} = 0.2s$, which has been confirmed by the discontinuousness of the first derivative of the ground-state energy.

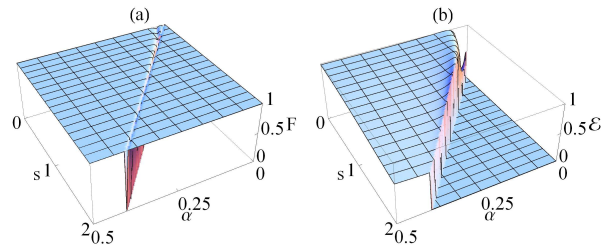


FIG. 2. (Color online) Ground state fidelity (a) and entanglement entropy (b) as a function of the coupling constant α and power index s of the spectrum. Here $\delta\alpha = 0.0005$, other parameters used here are the same as Fig. 1. The singularity near the critical point $\alpha_{\text{C,RWA}}$ of forming bound state shows existence of QPT in this model.

for the spectral density (2).

B. Numerical results

To verify the existence of QPT in the model quantitatively, in the following we study numerically the ground-state energy and its derivative, fidelity and entanglement entropy of the ground state near the critical point with the change of the coupling constant of the system.

At zero temperature, the non-analyticity of the ground-state energy is directly connected to the QPT. The first (or n -th) order QPT is characterized by the discontinuity in the first (or n -th) derivative of the ground state energy. In Fig. 1, we plot the ground state energy and its first derivative. It can be seen that the first derivative is discontinuous at the critical point (7), which means that it is a first-order QPT.

The QPT can be further verified by the fidelity F and entanglement entropy \mathcal{E} between the TLS and the reservoir of the ground state. The ground-state fidelity is defined as the overlap of two ground states corresponding to two slightly different control parameters [32], i.e. $F = \langle \varphi_g(\alpha) | \varphi_g(\alpha + \delta\alpha) \rangle$. The entanglement entropy can be obtained by calculating the entropy of the reduced density matrix of the TLS after tracing out the reservoir de-

degrees of freedom. In Fig. 2(a), we plot F near the critical point. The singularity in the plot evidences clearly the existence of QPT in this model. Because of the totally orthogonal property of ground state, the fidelity completely drops to zero at the critical point. In Fig. 2(b), we plot \mathcal{E} of the ground state. Near the critical point, we find a sudden birth of the ground-state entanglement, which can be seen as a result of changing of ground-state structure. This discontinuousness in the ground-state entanglement entropy also evidences the existence of QPT.

IV. QPT WITHOUT THE RWA

In the following, using the perturbation approach based on unitary transformation [5, 6], we study whether or not the QPT still occurs when the RWA is relaxed.

A. Analytical results

A unitary transformation $\hat{U}_2 = \exp[\sum_k \frac{g_k \xi_k}{2\omega_k} (\hat{b}_k^\dagger - \hat{b}_k) \hat{\sigma}_x]$ can recast Eq. (3) into

$$\begin{aligned} \hat{H}' = & \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k \frac{g_k(1-\xi_k)}{2} (\hat{b}_k + \hat{b}_k^\dagger) \hat{\sigma}_x \\ & + \frac{\Delta}{2} [\hat{\sigma}_z \cosh \hat{\chi} - i \hat{\sigma}_y \sinh \hat{\chi}] + C, \end{aligned} \quad (8)$$

where $C = \sum_k \frac{g_k^2}{4\omega_k} \xi_k (\xi_k - 2)$, $\hat{\chi} = \sum_k \frac{g_k \xi_k}{\omega_k} (\hat{b}_k^\dagger - \hat{b}_k)$, and ξ_k are to be determined. We can further separate \hat{H}' into

$$\hat{H}' = \hat{H}'_0 + \hat{V}', \quad (9)$$

where

$$\begin{aligned} \hat{H}'_0 = & \frac{\eta \Delta}{2} \hat{\sigma}_z + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + C, \\ \hat{V}' = & \sum_k \frac{g_k(1-\xi_k)}{2} (\hat{b}_k + \hat{b}_k^\dagger) \hat{\sigma}_x - i \frac{\Delta}{2} \hat{\sigma}_y \sinh \hat{\chi} \\ & + \frac{\Delta}{2} \hat{\sigma}_z (\cosh \hat{\chi} - \eta), \end{aligned} \quad (10)$$

with

$$\eta = \langle \{0_k\} | \cosh \hat{\chi} | \{0_k\} \rangle = \exp[-\sum_k \frac{g_k^2 \xi_k^2}{2\omega_k^2}]. \quad (11)$$

We can see from Eq. (9) that, to the zero-order approximation, the spin-boson interactions can be eliminated to generate an effective noninteracting Hamiltonian characterized by a renormalized tunneling amplitude $\Delta_{eff} \equiv \eta \Delta$ with η as renormalized factor.

With the separation of Eq. (9), we can readily calculate the Bogoliubov-Peierls bound on the free energy F_B of the system [33]. The free energy F of the system is related to F_B by $F \leq F_B$ with

$$F_B = -\beta^{-1} \ln \text{Tr} \exp(-\beta \hat{H}'_0) + \langle \hat{V}' \rangle_{\hat{H}'_0}, \quad (12)$$

where $\beta = \frac{1}{k_B T}$, $\langle \cdot \rangle_{\hat{H}'_0}$ denotes the thermal expectation value calculated with respect to \hat{H}'_0 , and the trace is calculated using the eigenstates of \hat{H}'_0 . It is easy to find $\langle \hat{V}' \rangle_{H_0} = 0$. Therefore,

$$F_B = F_{\text{Boson}} - \frac{\ln[2 \cosh \frac{\beta \Delta \eta}{2}]}{\beta} + C. \quad (13)$$

The parameters ξ_k are determined by minimizing F_B with respect to ξ_k , that is $\frac{\partial F_B}{\partial \xi_k} = 0$. We find in our zero-temperature case (i.e. $\beta \rightarrow \infty$)

$$\xi_k = \frac{\omega_k}{\omega_k + \eta \Delta}. \quad (14)$$

By now, the parameters ξ_k as well as the renormalized factor η have been determined. The renormalized factor η has been used successfully to characterize the delocalized-localized QPT in the SBM [5, 6, 17]. If the tunneling amplitude is renormalized to zero, the system is in the localized phase and the dynamics is trivial. In contrast, if the renormalized tunneling amplitude is nonzero, then the system is in the delocalized phase, which displays some interesting dynamical behaviors such as damped coherent oscillation and incoherent relaxation.

Focusing on the delocalized phase regime, we further separate the first-order perturbation term from $\hat{V}' = \hat{H}'_1 + \hat{H}'_2$ with

$$\begin{aligned} \hat{H}'_1 = & \sum_k \frac{g_k(1-\xi_k)}{2} (\hat{b}_k + \hat{b}_k^\dagger) \hat{\sigma}_x - i \frac{\Delta \eta}{2} \hat{\sigma}_y \hat{\chi} \\ = & \sum_k \nu_k (\hat{b}_k \hat{\sigma}_+ + \hat{b}_k^\dagger \hat{\sigma}_-), \\ \hat{H}'_2 = & \frac{\Delta}{2} \hat{\sigma}_z (\cosh \hat{\chi} - \eta) - i \frac{\Delta}{2} \hat{\sigma}_y (\sinh \hat{\chi} - \eta \hat{\chi}), \end{aligned} \quad (15)$$

where $\nu_k = \eta \Delta g_k \xi_k / \omega_k$ and $\hat{\sigma}_\pm = (\sigma_x \pm i \sigma_y)/2$. Combined with Eq. (9), we arrive at the transformed SBM as $\hat{H}' = \hat{H}'_0 + \hat{H}'_1 + \hat{H}'_2$, where \hat{H}'_0 collects all the renormalized non-interacting terms, \hat{H}'_1 collects all the first-order perturbation terms, and \hat{H}'_2 collects all the higher-order perturbation ones. It means that by appropriately choosing the unitary transformation, we can separate automatically the excitation-conservative transition terms \hat{H}'_0 and \hat{H}'_1 from the multi-boson-excitation and nondiagonal transition \hat{H}'_2 . It has been proved that in zero-temperature and weak coupling (i.e. the delocalized) regimes the higher-order perturbation terms \hat{H}'_2 can be neglected [6]. Then the transformed Hamiltonian has the form $\hat{H}' \approx \hat{H}'_0 + \hat{H}'_1 \equiv \hat{H}_{\text{eff}}$

$$\hat{H}_{\text{eff}} = \frac{\Delta \eta}{2} \hat{\sigma}_z + \sum_k [\omega_k \hat{b}_k^\dagger \hat{b}_k + \nu_k (\hat{b}_k^\dagger \hat{\sigma}_- + \hat{b}_k \hat{\sigma}_+)] + C \quad (16)$$

which shares the formal similarity with the rotating-wave approximate Hamiltonian (4).

With the similar procedure as in Sec. III and neglecting temporarily the constant term C in Eq. (16), we

can determine that a bound state $|\varphi'_1\rangle = d_0|+\rangle + \sum_k d_k|-\rangle$ with the eigenvalue E_1 satisfying

$$y(E_1) \equiv \frac{\eta\Delta}{2} - \sum_k \frac{\nu_k^2}{\omega_k - (E_1 + \frac{\eta\Delta}{2})} = E_1 \quad (17)$$

can be formed for \hat{H}_{eff} . This equation permits a real root in the regime $E_1 \leq -\eta\Delta/2$ if and only if $y(-\eta\Delta/2) \leq -\eta\Delta/2$. Accompanying with the formation of a bound state, the ground state is changed from $|\varphi'_0\rangle \equiv |-\rangle$ to $|\varphi'_1\rangle$. Recovering back the neglected term C , we get the ground-state energy as

$$E_g = \begin{cases} -\frac{\eta\Delta}{2} - C, & \alpha < \alpha_c \\ E_1 - C, & \alpha > \alpha_c \end{cases} \quad (18)$$

where the critical point α_c can be determined by solving equation $y(-\eta\Delta/2) = -\eta\Delta/2$. Physically, such a sudden change of the ground-state structure signals clearly the occurrence of QPT in the system.

It is noted that the neglected higher-order perturbation term \hat{H}'_2 gives no contribution to the QPT because it is zero, i.e. $\langle\varphi'_i|\hat{H}'_2|\varphi'_j\rangle = 0$ ($i, j = 0, 1$), in the two eigen bases. It means that the neglected term \hat{H}'_2 has no impact on such level-crossing-caused QPT. This in turn validates our approximation.

B. Numerical results

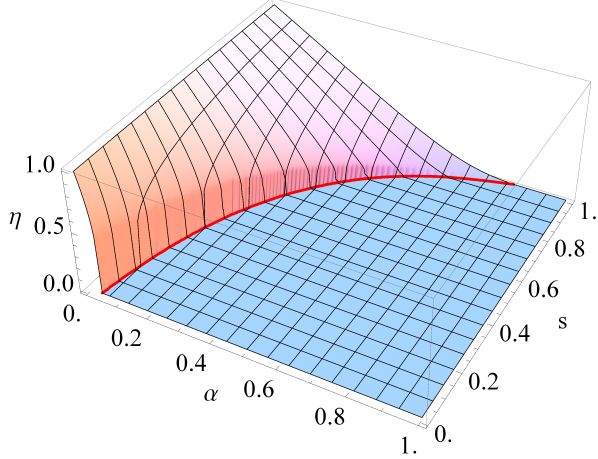


FIG. 3. (Color online) The conventional delocalized-localized QPT characterized by the renormalized factor η as a function of the coupling constant α and the power index s of the spectrum. The red solid line depicts the critical point. $\Delta = 0.1\omega_c$ has been used in the numerical calculation.

For completeness, we firstly recover the conventional delocalized-localized QPT in the full range of the sub-Ohmic spectral density. In Fig. 3, we plot the numerical results on this conventional QPT characterized by η ,

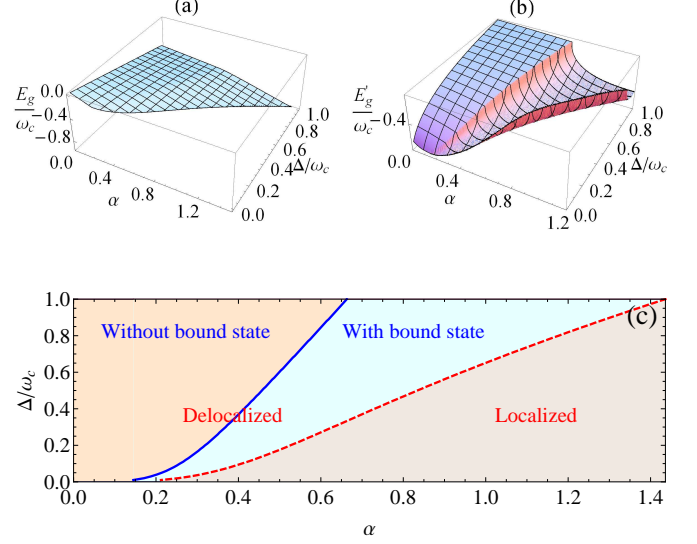


FIG. 4. (Color online) (a): Ground-state energy E_g and (b): its first derivative $E'_g = \frac{\partial E_g}{\partial \alpha}$ as a function of α and Δ , and (c): the phase diagram when $s = 0.8$. The red dashed line and the blue solid line mark the critical points of the conventional delocalized-localized QPT and the novel bound state QPT, respectively.

which can be calculated by solving Eqs. (11) and (14) self-consistently. We can see that the system is in the delocalized phase regime when α is small, where η takes a finite value. With the increase of α , η drops suddenly to zero and the system enters into the localized phase regime. Such delocalized-localized QPT is present in the whole range of the power index s of the sub-Ohmic spectral density. This is coincident with the results under the quantum Monte Carlo method and the numerical diagonalization method [8, 9]. The critical point of this QPT tends to $\alpha_c = 1$ with the increase of s to Ohmic case. This is consistent with the well-known results that the delocalized-localized phase transition occurs at $\alpha_c = 1$ in the small Δ limit for the Ohmic SBM [4].

Focusing explicitly on the conventional delocalized phase regime, where η takes a finite value, we now study the ground state energy of the sub-Ohmic SBM. From the analysis above, we know that the formation of a bound state in the single-excitation subspace of \hat{H}_{eff} causes the level crossing of the ground state, which triggers a novel QPT to the model. To verify this, taking $s = 0.8$ as an example, we plot in Fig. 4(a) and (b), respectively, the ground state energy and its first derivative to the coupling constant according to Eq. (18). We can see that E_g is continuous, but $\frac{dE_g}{d\alpha}$ shows a discontinuity at the critical point α_c where the bound state is formed. It manifests clearly that there is another QPT existing in the delocalized phase regime. In Fig. 4(c) the phase diagram is depicted. It indicates that besides the conventional delocalized-localized QPT with the critical point

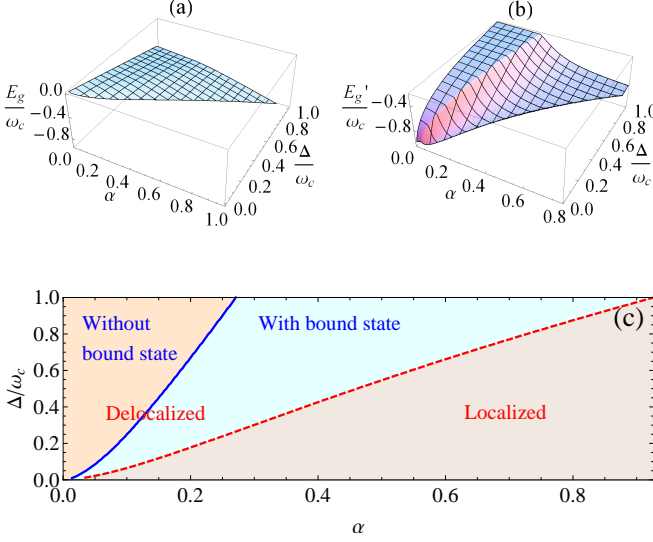


FIG. 5. (Color online) (a): Ground-state energy E_g and (b): its first derivative $E'_g = \frac{\partial E_g}{\partial \alpha}$ as a function of α and Δ , and (c): the phase diagram when $s = 0.4$. The red dashed line and the blue solid line mark the critical points of the conventional delocalized-localized QPT and the novel bound state QPT, respectively.

marked by the red dashed line, there is another novel QPT with the critical point marked by the blue solid line occurring in the delocalized phase regime. To check if such novel QPT is also present in $0 < s < 1/2$, where the quantum-classical mapping was proven to be breakdown by the numerical renormalization group method [7], we take $s = 0.4$ as an example and plot explicitly the ground state energy, its derivative, and the phase diagram in Fig. 5. We can see although the delocalized phase regime much shrinks with the decrease of s , it still separates into two further regimes with and without the bound state. It shows that the novel QPT also shows up when $0 < s < 1/2$.

V. DYNAMICAL CONSEQUENCES OF THE QPT

To evaluate the consequences of the novel QPT on the non-equilibrium dynamics of the spin system, we study next the evolution of the spin system under certain initial condition. It has been found that the spin dynamics shows the so-called coherent-incoherent transition [4] in the delocalized phase regime when the initial state of the reservoir is in vacuum [15, 16]. Some theoretical [22–27] and experimental [28–30] works also show that the dynamics of the SBM under the RWA exhibits rich dynamics, from complete decoherence to decoherence suppression. We argue that both of the two different dynamical behaviors are essentially caused by a same reason, i.e.

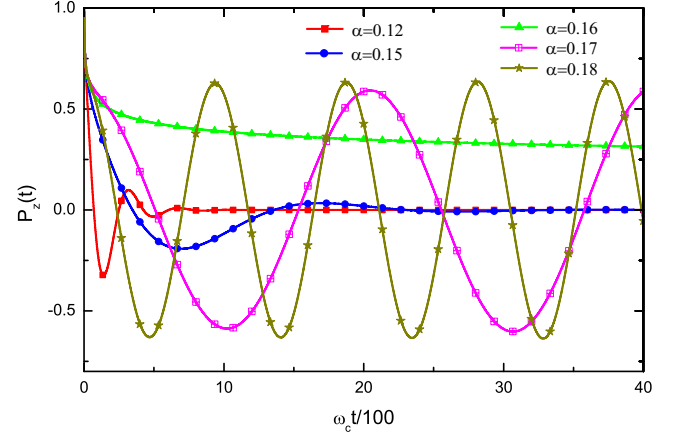


FIG. 6. (Color online) The nonequilibrium dynamics of $P_z(t)$ of the SBM with the RWA under the initial condition Eq. (19). Here the parameters $s = 0.8$ and $\Delta = 0.1\omega_c$ have been used. Consequently, the critical point is $\alpha_{C,RWA} = 0.16$.

the novel QPT we revealed in Sec. III with the RWA and the in Sec. IV without the RWA. To verify this, we study in the following the dynamics of the SBM both with and without the RWA.

Firstly, we study the nonequilibrium dynamics of the spin under the RWA. Assuming initially the whole system is in

$$|\Psi_1(0)\rangle = |+, \{0_k\}\rangle, \quad (19)$$

which, in the \hat{H}_z , i.e. Eq. (3), representation, takes the form as $|\Psi_z(0)\rangle = \hat{U}_1|\Psi_1(0)\rangle = |+_x, \{0_k\}\rangle$ with $|+_x\rangle$ satisfying $\hat{\sigma}_x|+_x\rangle = |+_x\rangle$. The time evolution of $|\Psi_z(0)\rangle$ is governed by Eq. (4) under the RWA. Therefore, the time-dependent solution can be expanded as

$$|\Psi_z(t)\rangle = e^{i\frac{\Delta t}{2}} \left[\frac{1}{\sqrt{2}} |-, 0_k\rangle + c(t) |+, 0_k\rangle + \sum_k d_k(t) |-, 1_k\rangle \right]. \quad (20)$$

From the Schrödinger equation, we can get the probability amplitude $c(t)$ satisfying

$$\dot{c}(t) + i\Delta c(t) + \int_0^t f(t-\tau)c(\tau)d\tau = 0, \quad (21)$$

where the kernel function $f(t-\tau) \equiv \frac{1}{4\pi} \int_0^{+\infty} J(\omega)e^{-i\omega(t-\tau)}d\omega$ and the initial condition $c(0) = 1/\sqrt{2}$. With this result at hands, we can calculate $P_z \equiv \langle \Psi(0) | e^{i\hat{H}t} \hat{\sigma}_z e^{-i\hat{H}t} | \psi(0) \rangle$ under the RWA as

$$P_z(t) = \langle \Psi_z(t) | \hat{\sigma}_x | \Psi_z(t) \rangle = \sqrt{2} \text{Re}[c(t)]. \quad (22)$$

In Fig. 6 we plot $P_z(t)$ of Eq. (22) in different coupling constants. According to Eq. (7), the QPT occurs at $\alpha_{C,RWA} = 0.16$. We can see that the dynamics reduces the oscillatory damping to zero when $\alpha < 0.16$. It is understandable from the fact that the bound state in this

region is absent and all the quantum coherence decays to zero. We call the character of the dynamics in this region as the complete decoherence. When $\alpha = 0.16$, it is very interesting to find that the coherence does not decay to zero and a finite quantum coherence is preserved in the steady state. In this situation, the bound state $|\varphi_1\rangle$ with the eigenvalue being just $E_1 = -\Delta/2$, which is equal to E_0 , is formed. As a stationary state, the quantum coherence contributed from the component $|\varphi_1\rangle$ to Eq. (19) does not change during the time evolution. Therefore, we get a finite asymptotical $P_z(t)$. With the further increase of α , the dynamics shows lossless oscillation. The bound state with smaller eigenvalue than E_0 is present. In this region, the components of $|\varphi_0\rangle$ and $|\varphi_1\rangle$ in Eq. (19) have different time dependence. The difference of the two eigenvalues, i.e. $E_0 - E_1$, contributes to the frequency of this lossless oscillation. A larger α induces a smaller E_1 and a more faster oscillation of $P_z(t)$. We call the character of the dynamics in the region $\alpha \geq \alpha_{\text{C,RWA}}$ as the decoherence suppression.

Next, we study the dynamics when the RWA is relaxed. To make the dynamics manifest the effect of the formed bound state exclusively, we choose the initial state as

$$|\Psi_2(0)\rangle = |+\rangle \otimes \hat{U}_2^\dagger |\{0_k\}\rangle. \quad (23)$$

It is noted that this state is different from Eq. (19), under which it has been shown that the dynamics of the SBM without the RWA exhibits the coherent-incoherent transition. The merit of choosing this state as the initial state is that it takes the form as $|\Psi(0)\rangle = \hat{U}_2 \hat{U}_1 |\Psi_2(0)\rangle = |+_x, \{0_k\}\rangle$ in the \hat{H}_{eff} representation. Therefore, besides the zero-excitation, only the single-excitation subspace where the bound state is formed is involved in the dynamics. In the same manner as the above RWA case, we can calculate $P_z(t) = \sqrt{2}\text{Re}[h(t)]$, where $h(t)$ satisfying

$$\dot{h}(t) + i\eta\Delta h(t) + \int_0^t f'(t-\tau)h(\tau)d\tau = 0, \quad (24)$$

with the initial condition being $h(0) = \frac{1}{\sqrt{2}}$ and the kernel function $f'(t-\tau) \equiv \frac{1}{4\pi} \int_0^\infty J'(\omega)e^{-i\omega(t-\tau)}d\omega$ connecting to the renormalized spectral density $J'(\omega) = \sum_k \nu_k^2 \delta(\omega - \omega_k)$.

Fig. 7 portrays $P_z(t)$ under the initial condition (23) when the RWA is relaxed. We can see that the similar behavior as Fig. 6 is present. When $\alpha < \alpha_{\text{C}}$, the bound state is absent. Therefore, the dynamics shows complete decoherence with the quantum coherence decaying to zero. When $\alpha = \alpha_{\text{C}}$, a finite steady $P_z(t)$ can be obtained asymptotically due to the double degeneracy of $|\varphi'_0\rangle$ and the formed bound state $|\varphi'_1\rangle$. When $\alpha > \alpha_{\text{C}}$, $P_z(t)$ shows decoherence suppression with the quantum coherence tending to lossless oscillation, where the frequency of this oscillation is determined by the difference between the two eigenvalues of $|\varphi'_0\rangle$ and $|\varphi'_1\rangle$.

From the analysis above, we can see that the novel QPT induced by the formation of the bound state has

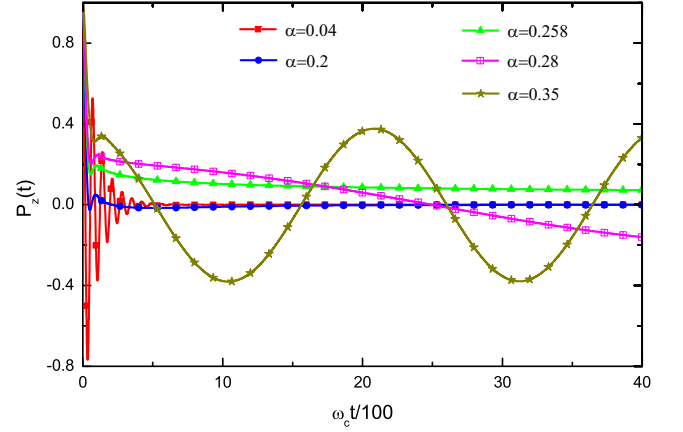


FIG. 7. (Color online) The nonequilibrium dynamics of $P_z(t)$ of the SBM without the RWA under the initial condition Eq. (23). Here the parameters $s = 0.8$ and $\Delta = 0.1\omega_c$ have been used. The critical point can be evaluated numerically at $\alpha_{\text{C}} = 0.258$.

a profound consequence to the nonequilibrium dynamics of the TLS in the conventional delocalized phase regime. It induces a dynamical transition from complete decoherence to decoherence suppression for the initial states where only the single-excitation subspace is involved. On the other hand, a widely studied case is the nonequilibrium dynamics of the TLS when the reservoir is initially in a vacuum state, where the spin dynamics shows a transition from damped coherent oscillation to incoherent relaxation, i.e. the so-called coherent-incoherent transition, in the delocalized-phase-regime. Therefore, it is reasonable to conjecture that the coherent-incoherent transition is also a dynamical consequence of this novel QPT on the initial vacuum state of the reservoir. This has been proved analytically for the Ohmic spectral density in Ref. [18] that α_{C} of the QPT matches well with the point of the coherent-incoherent transition. Thus, we can conclude that both of the transitions from complete decoherence to decoherence suppression and from damped coherent oscillation to incoherent relaxation are actually the different dynamical consequences of the same intrinsic QPT on different initial states.

VI. CONCLUSION

In conclusion, we have studied the QPT of sub-Ohmic SBM both with and without RWA. When the RWA is used, we reveal that a novel QPT induced by the formation of a bound state in the single-excitation subspace occurs, while the delocalized-localized QPT is absent. When the RWA is relaxed, we first obtain that the conventional delocalized-localized QPT occurs in the whole range of the sub-Ohmic spectrum, which is consistent with the results under the quantum Monte Carlo method and the numerical diagonalization method [8, 9]. Then

using the perturbation approach to neglect the high-order interaction terms in unitarily transformed Hamiltonian, we show that the bound-state-induced QPT still exists in delocalized phase regime. The approximation is justified by that we are working in the weak coupling (i.e. the delocalized phase) regime and in the zero-temperature case, where the high-order excitations are negligible. On the other hand, one also can verify that the neglected terms give no contribution to the QPT we obtained, which in turn validates our approximation. We also have studied the dynamical consequences of the novel QPT. It is shown that the QPT causes a dynamical transition from complete decoherence to decoherence suppression to the initial state in which only the single-excitation subspace is involved. This result is compatible to the coherent-incoherent transition which happens to the state where the reservoir is initially in vacuum. It conjectures that the coherent-incoherent transition reported in the literature is essentially caused by the intrinsic QPT of the SBM.

As a final remark, the results obtained in the present work is only in the un-biased SBM, i.e. $\epsilon = 0$. It is also interesting to generalize our discussions to the biased case. This work is in progress.

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Appendix A: The bound state with higher-excitation

The eigenstate of \hat{H}_{eff} with $N = 2$ can be expanded as

$$|\varphi_2\rangle = \sum_k (d_k|+, 1_k\rangle + e_k|-, 2_k\rangle + \sum_{k' \neq k} f_{k,k'}|-, 1_k, 1_{k'}\rangle). \quad (\text{A1})$$

From the eigen equation $\hat{H}_{\text{eff}}|\varphi_2\rangle = E_2|\varphi_2\rangle$, we obtain the following coupled equations

$$E_2 d_k = \left(\frac{\eta\Delta}{2} + \omega_k\right) d_k + \sqrt{2}\nu_k e_k + \sum_{k' \neq k} \nu_{k'} f_{k,k'}, \quad (\text{A2})$$

$$E_2 e_k = \sqrt{2}\nu_k d_k + (2\omega_k - \frac{\eta\Delta}{2}) e_k, \quad (\text{A3})$$

$$E_2 f_{k,k'} = \nu_{k'} d_k + (\omega_k + \omega_{k'} - \frac{\eta\Delta}{2}) f_{k,k'}. \quad (\text{A4})$$

Substituting the solutions of Eqs. (A3) and (A4) in term of d_k into Eq. (A2), we have

$$E_2 = \frac{\eta\Delta}{2} + \omega_k + \frac{\nu_k^2}{E_2 - (-\frac{\eta\Delta}{2} + 2\omega_k)} + \sum_{k'} \frac{\nu_{k'}^2}{E_2 - (-\frac{\eta\Delta}{2} + \omega_k + \omega_{k'})}. \quad (\text{A5})$$

Generally, as the density of states per unit frequency is proportional to M , where M is the total number of bath oscillators, the microscopic coupling strengths have to scale as $M^{-1/2}$ in order to ensure that the spectral density is well defined in the thermodynamic limit. Therefore, in the thermodynamic limit, $M \rightarrow \infty$, ν_k itself is small [34], then Eq. (A5) reduces to

$$E_2 = \frac{\eta\Delta}{2} + \omega_k + \sum_{k'} \frac{\nu_{k'}^2}{E_2 - (-\frac{\eta\Delta}{2} + \omega_k + \omega_{k'})}. \quad (\text{A6})$$

Setting $E_2 = E'_2 + \omega_k$, we have

$$E'_2 = \frac{\eta\Delta}{2} - \sum_{k'} \frac{\nu_{k'}^2}{\omega_{k'} - (E'_2 + \frac{\eta\Delta}{2})}, \quad (\text{A7})$$

which is the same as Eq. (6) in the main text. It means

$$E'_2 = E_1 < E_2. \quad (\text{A8})$$

Therefore, even a bound state in the higher-excitation subspace can be formed, its eigenvalue is still larger than E_1 . This means that the higher-excitation bound state is not possible to be the ground state.

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